X-ray Studies of Shock Deformation of FCC Metals on Nanosecond Timescales

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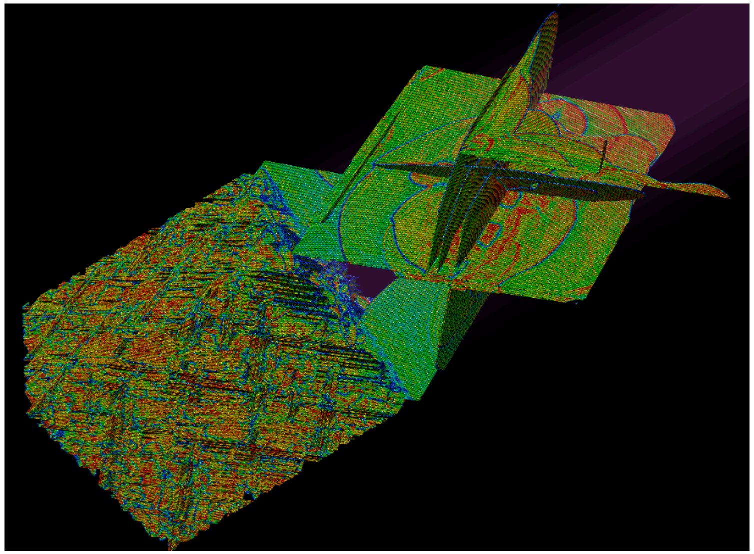
LLNL



Workshop on Time Domain Science
2004

Outline of Talk

- Introduction
- Experiments measuring lattice parameters of shocked silicon and copper
- MD Simulations
- Future Experiments
- Summary

Dynamic diffraction may resolve uniaxial vs. isotropic compression of the shocked lattice

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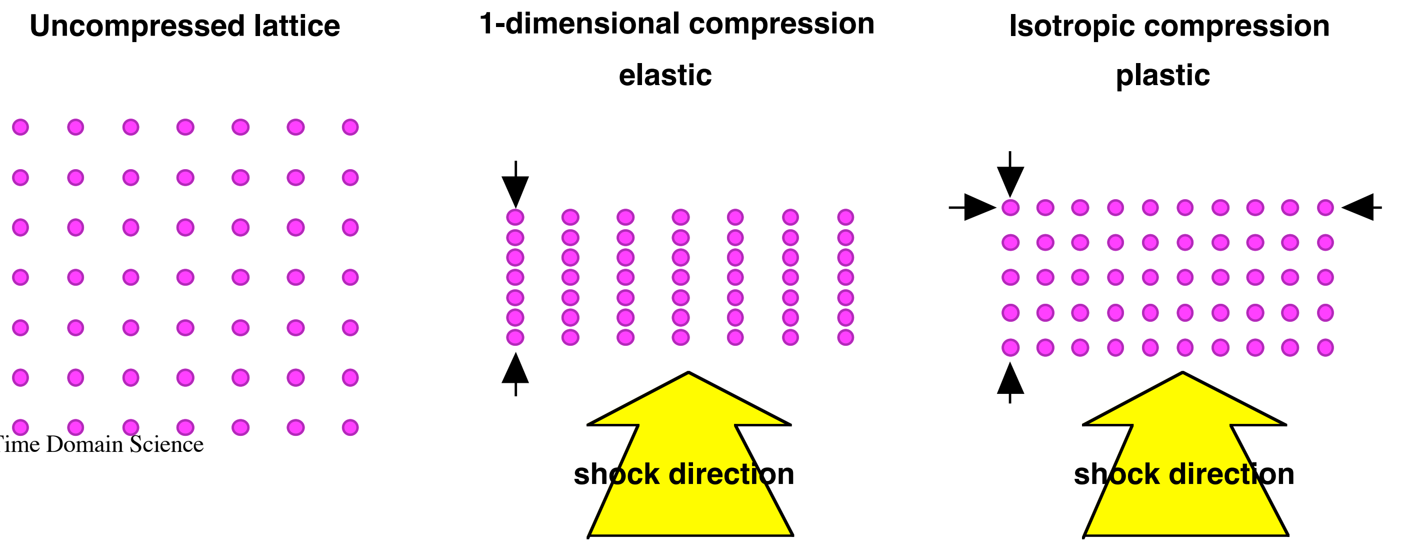
- Elastic compression is largely 1-dimensional
- Shock compression above the Hugoniot elastic limit (HEL) is plastic
- It is expected that the lattice rearranges to isotropic compression under plastic compression
- Dynamic Bragg diffraction may allow us to study the transition to plasticity



X-ray diffraction: principle of crystal structure determination

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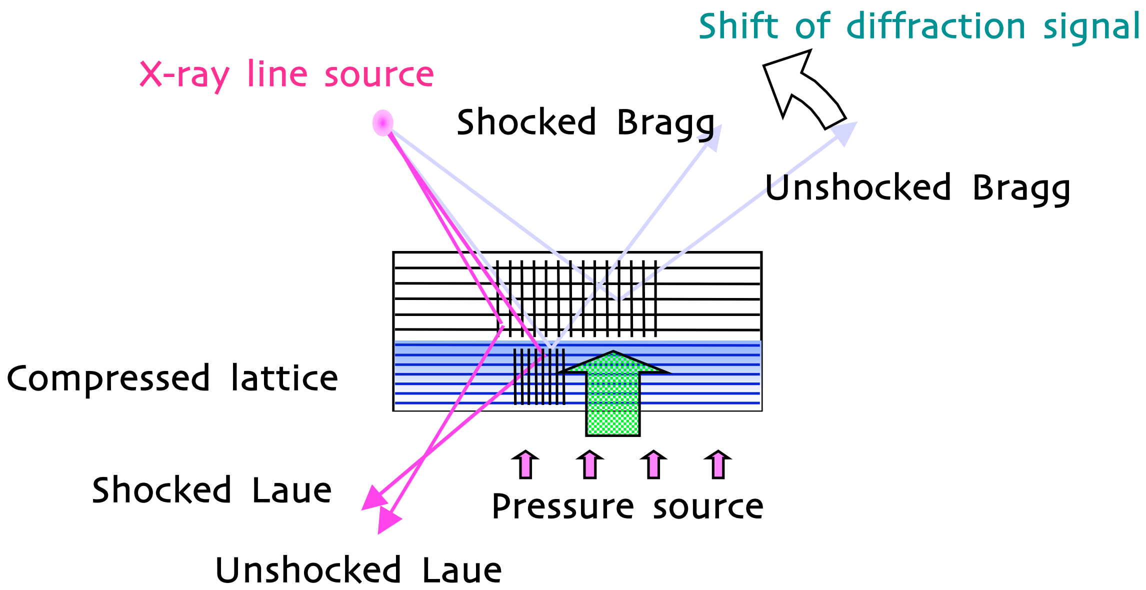
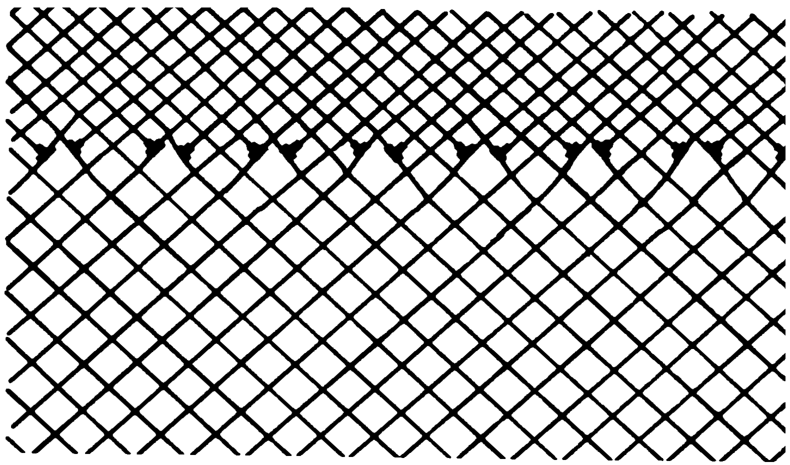
X-ray diffraction from shocked crystal



Dislocation generation model



- X-ray diffraction resolves uniaxial (elastic) compression and isotropic 3D compression beyond HEL threshold (plastic)
- Dislocation models predict cubic-to-cubic behaviour of shocked crystals [CS Smith, *Trans of Met. Soc. of AIME*, 1958; MA Meyers, *Scripta Metal.*, **12**, 1978]

‘Ultimate’ Strain Rate

Rate of plastic strain is determined by Orowan’s equation

$$\dot{\varepsilon} = Nbv$$

Estimate of maximum rate for copper at, say 5% strain. Distance between dislocations is 20 atoms, *b* ~2 Å, *v*~ 3kms^{-1}.

$$\dot{\varepsilon} \sim 10^{16} \times 2 \times 10^{-10} \times 3 \times 10^{3} = 6 \times 10^{9}$$

Timescale ~ 10 psec. Expected to be much longer for Silicon, as velocity is much lower.

Simultaneous measurement of (400) (Bragg) and (040) (Laue)

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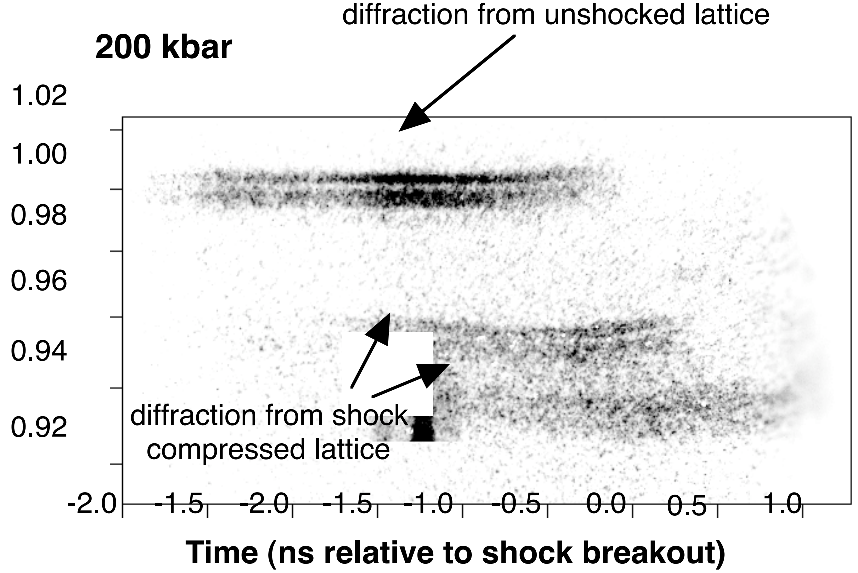
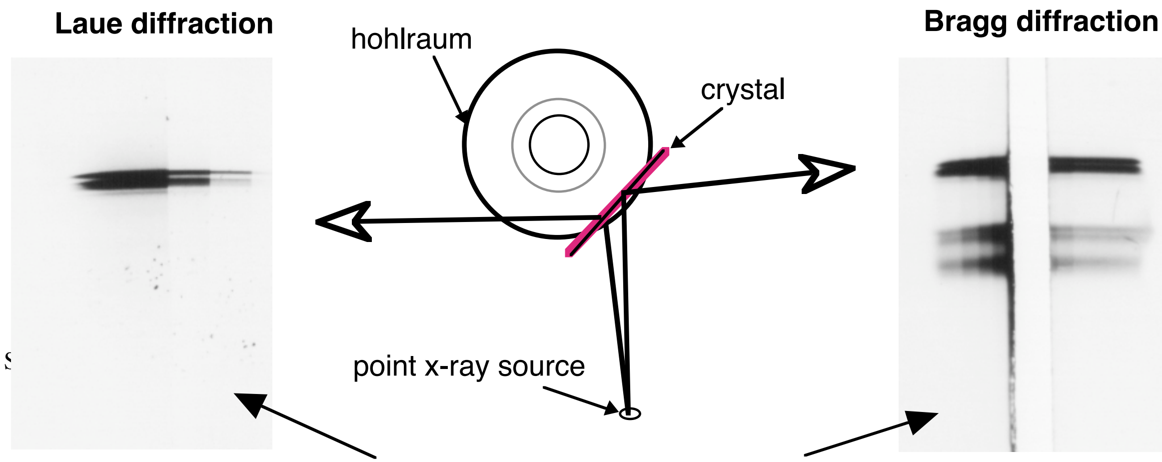
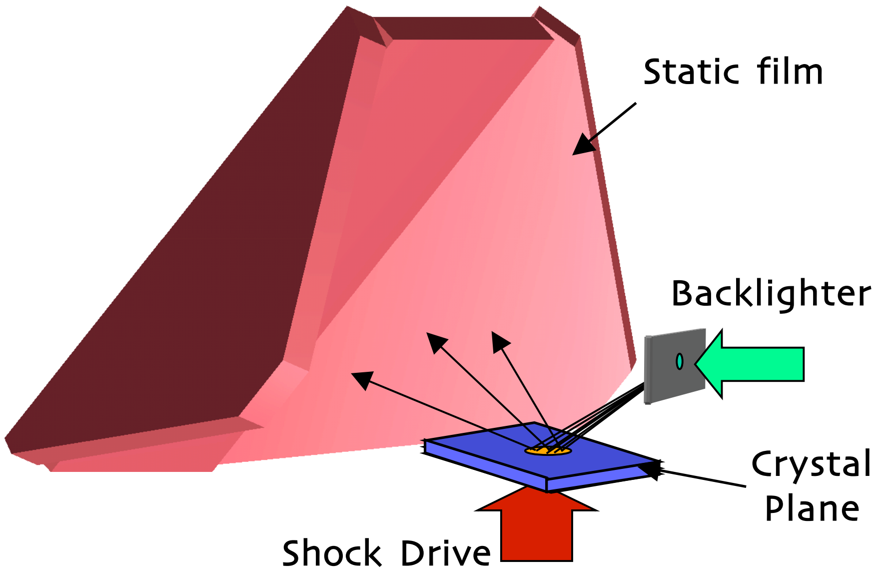
- Compression in (400) similar to (111) at the same drive
- Laue diffraction pattern shows uncompressed lattice





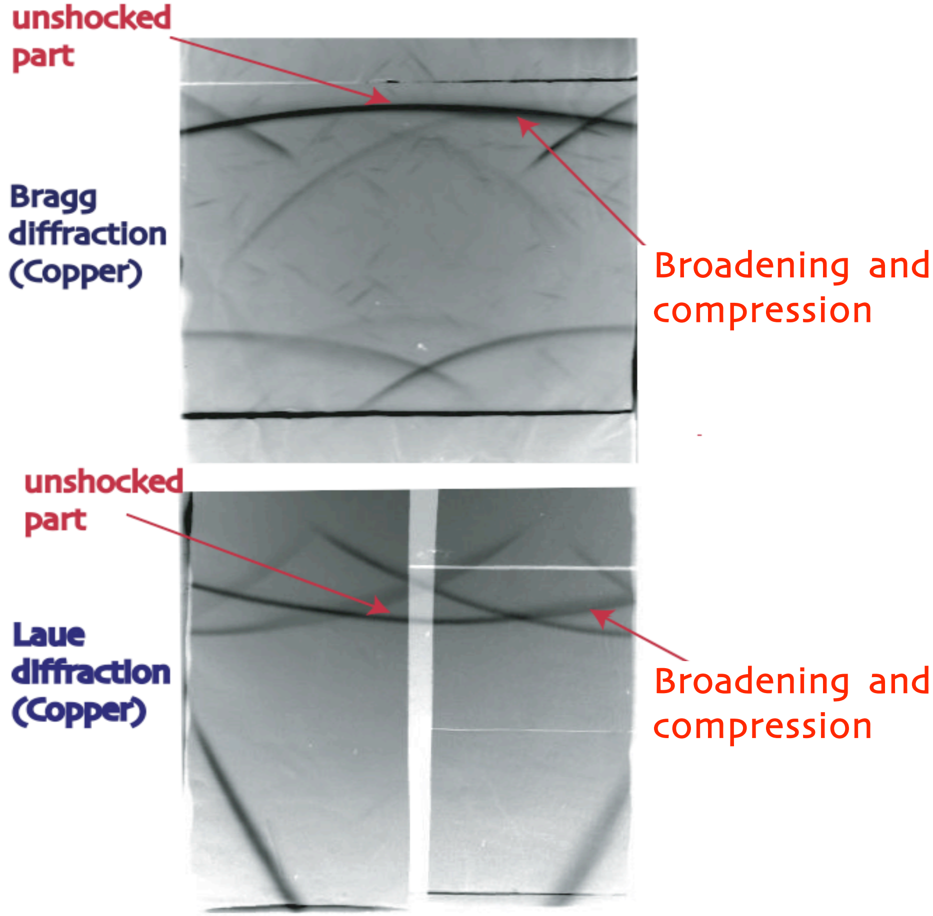
Experimental data using MFP

Wide angle film pack designed to detect multiple plane diffraction



[D.H.Kalantar et al., *Rev. Sci. Inst.*,**74**,2003]

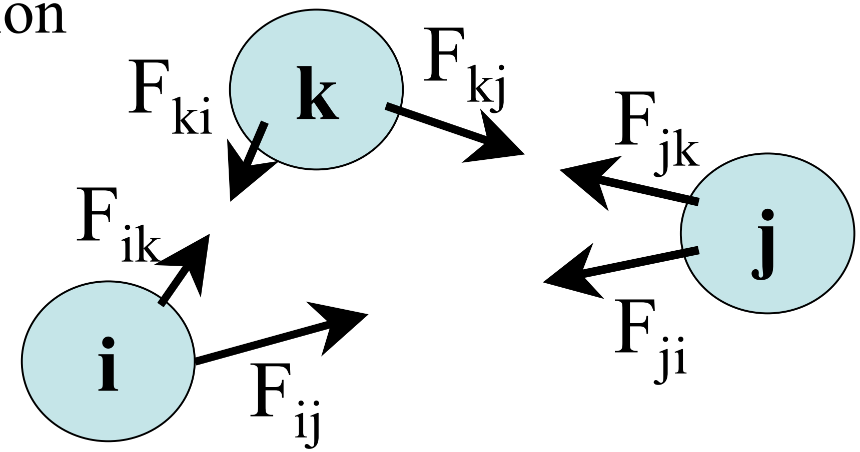
Recent Cu diffraction data (Vulcan)



Clear evidence of 3D compression

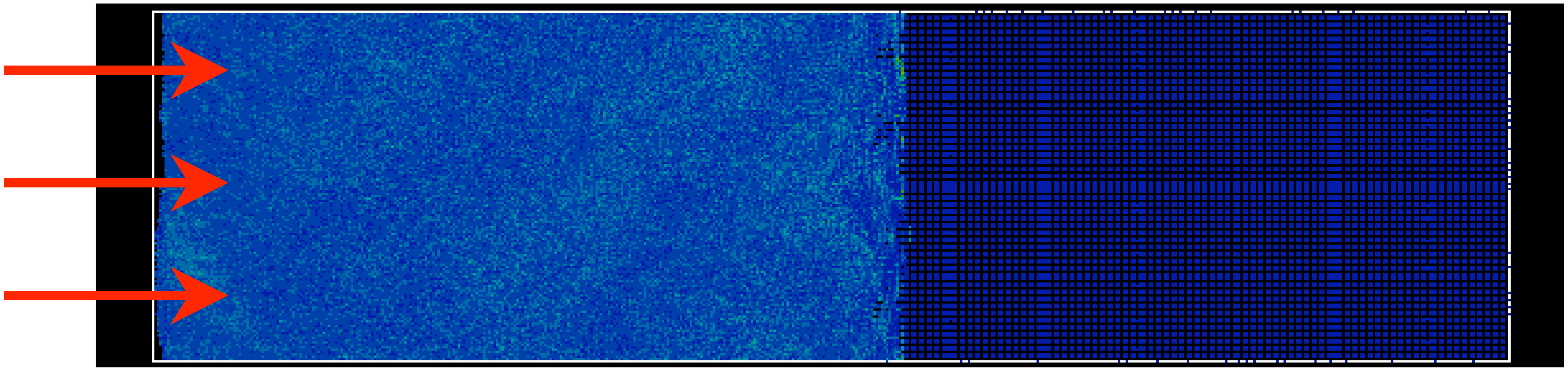
Classical Molecular Dynamics (MD) shock simulations

MD: Solve Newton's equations of motion for a system of atoms. Forces among atoms derived from empirical potential energy function (generally many-body terms, not just binary interactions).

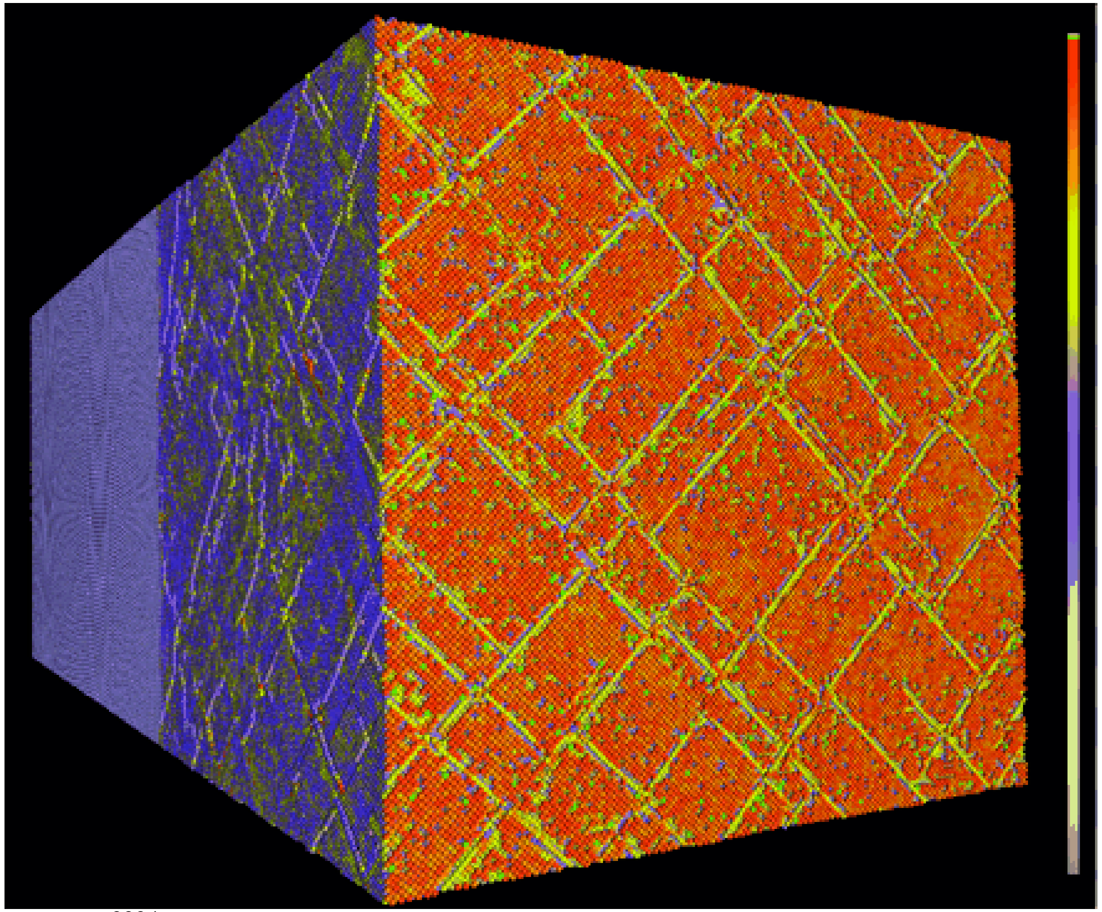


Shock Simulations

- 0.2-400 million atom simulations
- A force is applied to few atomic planes (the "piston") along desired shock direction, or the "piston" is moved at desired velocity



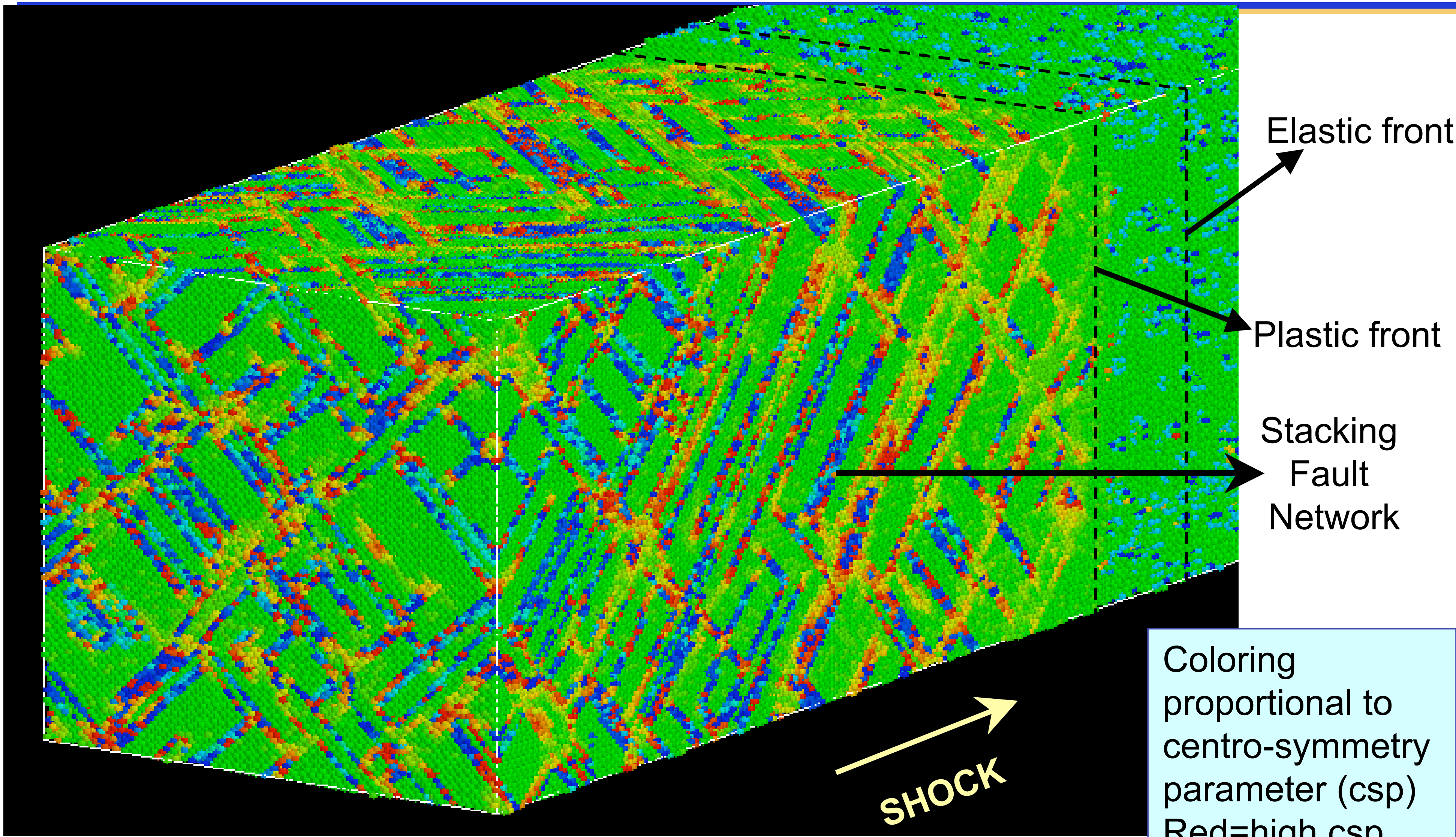
Molecular dynamics simulations of shocked fcc metals



Work by Brad Holian and coworkers at LANL shows that plasticity is caused by the homogeneous generation of stacking faults at the shock front on psec timescales in fcc metals.

B.L. Holian, P. Lomdahl, Science **280**, 2085 (1998)

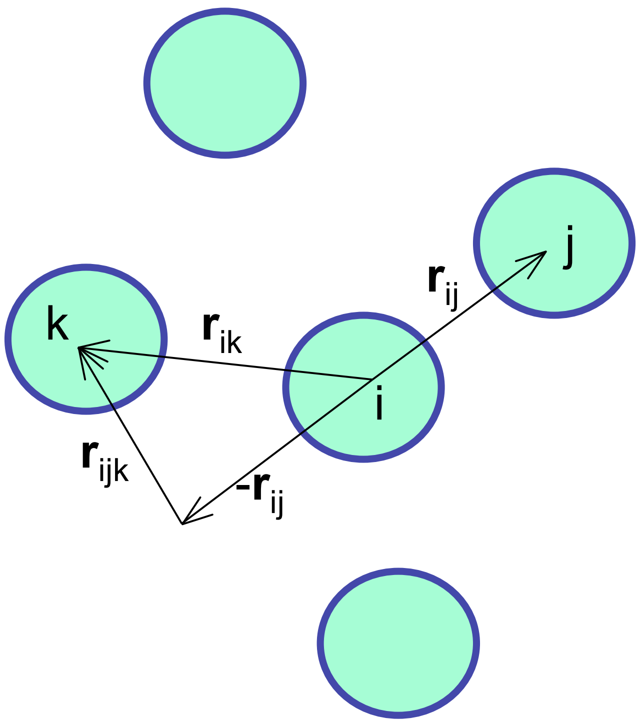
50 GPa shock along <100>, CSP analysis



Coloring proportional to centro-symmetry parameter (csp)
Red=high csp
Green=low csp

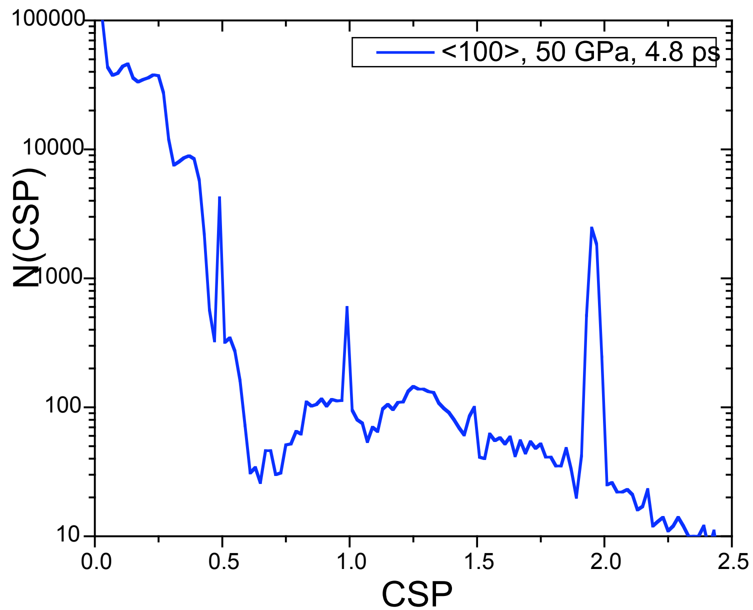
Centro Symmetry Parameter

$$\mathbf{csp(i)} = \Sigma_{NNi} \, |(r_{ik} - r_{ij})/a_o|^2 = \Sigma_{NNi} \, |r_{ijk}/a_o|^2$$



Kelchner, Plimpton and Hamilton,PRB **58** (1998) 11085
R. Rudd, J. Marian, W. Cai, E. Bringa

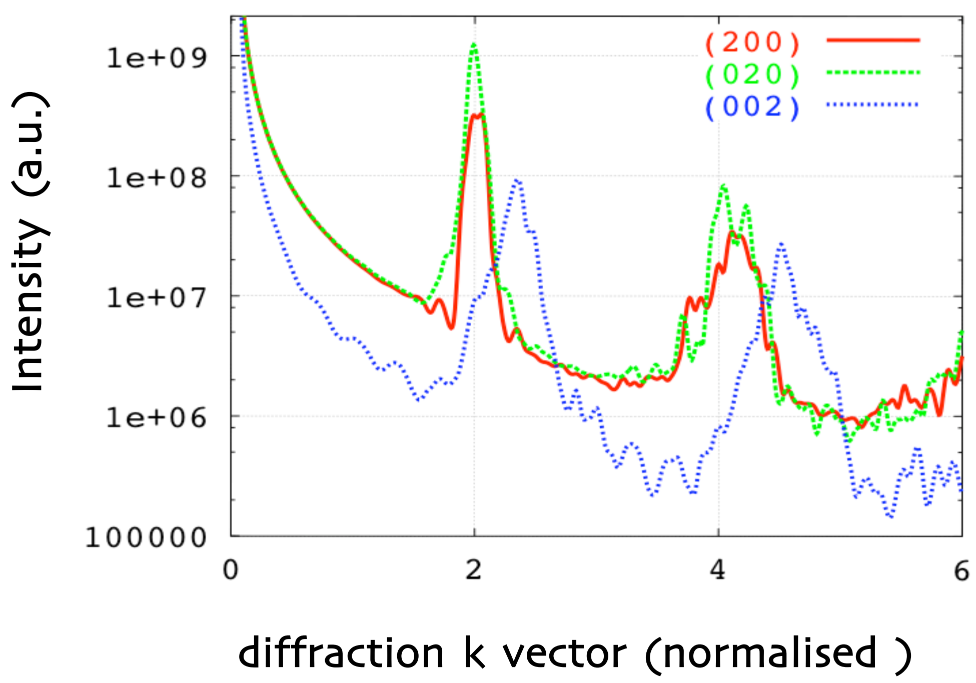
Perfect fcc crystal ⇒ csp(i) = 0
Crystal with defects ⇒ histogram



X-ray Diffraction Post-Processor Results: shock along <001>

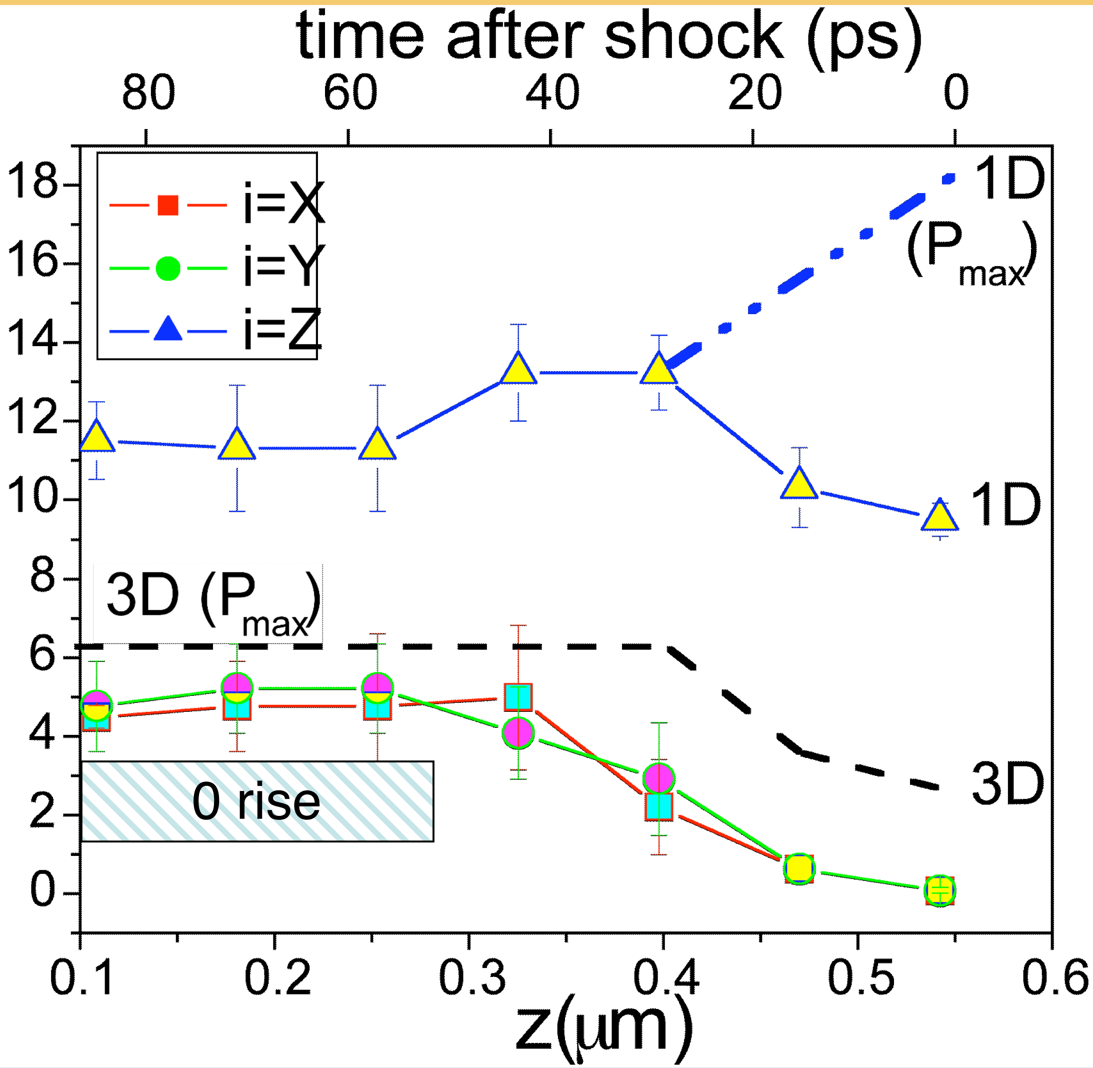
Oxford Physics

- **MD Sample size: 2×10^6 atoms**
- **Unit cell size normalised**
- **Pressure 50GPa**
- **'Zero' shock rise time**
- **Snapshot at 7.81 ps after start of shock**
- **EAM potential** [Y. Mishin et al., *PRB*, **63**, 2001]
- **Compression 18%**



• Detect 1D (~16.6 ±1.0%) compression along shock propagation direction; no detectable 3D compression in 2nd order

Is there 3D lattice deformation?



K. Rosolankova
J. Wark, Oxford

R. Frank (CASC)
Currently developing massively parallel X-ray tool (>10^8 atoms)

Large 3D deformation after ~60 ps:
50 ps rise time ➔~66% of full 3D; 0 rise time➔~50% of full 3D

Summary

- The large number of homogeneous dislocations get tangled - they cannot move quickly - therefore take time to relax to 3-D
- IF dislocation sources are activated before the main wave (i.e. a ramp of a few tens of ps), they can relieve shear stress with fewer, but more mobile dislocations.
- We predict that Cu will remain 1-D on a few ps timescale, even in the presence of dislocation sources, if the shock rise time is rapid.
- We further predict that homogeneous dislocation generation takes a few ps - before this the material behaves elastically.
- Picosecond diffraction experiments are required to resolve these issues + better materials characterization + more MD.